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COMMENTS OF SOVIET SCIENTIST ON 1953
PARIS CONFERENCE ON MOLECULAR STRUCTURE

[Comment: The following summary of an article by Academician B. A. Arbuzov on the 1953 Paris Conference on Molecular Structure reflects the viewpoint of Soviet scientists in general and that of Arbuzov in particular. Arbuzov tries to indicate that Soviet criticism of the resonance theory is in accord with tendencies prevalent in Western science.]

Two of the most important problems of modern theoretical chemistry are clarification of the nature of the chemical bond and elucidation of the connection between the structure of molecules and their physical properties, chemical behavior, and reactivity.

These problems command the attention not only of chemists, but also of physicists and biochemists. Investigation of the connection between the structure of molecules and their physiological activity is of great importance for biology in general and medicine in particular.

The second quarter of the 20th Century has been marked by considerable advances in the knowledge of the chemical bond. The application of the electron theory and of quantum mechanics has resulted in a greater understanding of the nature of the chemical bond and enabled us to explain the concepts and rules which had been formulated by chemists on the basis of an extensive accumulation of experimental material that was often purely empirical.

However, there is still no general agreement on the fundamental problems of theoretical chemistry: individual groups of scientists attempt to solve these problems starting from different concepts and using different methods. Thus, it is essential to discuss the fundamental postulates of contemporary chemistry from a broad standpoint, with participation not only of chemists but also of physicists and mathematicians.

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In recent years, a number of international meetings dealing with problems of the chemical bond have taken place. One meeting, organized by the French Physicochemical Society, was held in 1948. Another meeting devoted to problems in this field was held by the Royal Society of London in 1950. In 1951, a conference on the application of the methods of wave mechanics to the theory of valency took place in New York, and a conference was held in Moscow on the theory of the structure of organic compounds.

The Moscow conference was particularly interesting in regard to both the scope of the problems discussed and the principles guiding their discussion. The outstanding aspect of this conference was a discussion of the significance of A. M. Butlerov's theory of structure for present-day organic chemistry and also of the role played by the so-called resonance theory of L. Pauling and G. W. Wheland and the theory of mesomerism of K. Ingold.

During the past 15-20 years, the theory of resonance has been widely accepted by foreign chemists and by some Soviet chemists. There has been a tendency to put this theory in the foremost place in organic, physical, and inorganic chemistry and thus to replace the classical structural theory of Butlerov with the theory of resonance. During the discussions held at the Moscow conference, the harmful character and idealistic nature of the theory of resonance were definitely exposed, while the continuing validity of Butlerov's theory was confirmed.

In the light of the decisions of the Moscow conference, the meeting held on 4-10 July 1953 by the French Physicochemical Society was of especial interest. The program of this meeting, which was at the same time a regular annual meeting of the society, consisted of a review of progress in the knowledge of the chemical bond and of a discussion of individual physical methods applied to the determination of the structure of molecules. In addition to French scientists, prominent chemists from Great Britain, West Germany, the USSR, and the US participated in the meeting. Representing the USSR were N. V. Belov, B. A. Arbuzov, P. P. Shorygin, and B. M. Kozyrev.

The meeting was conducted in a businesslike manner. After the opening address, "Progress in the Knowledge of the Nature of the Chemical Bond," by Professor E. Boyer, Professor H. C. Longuet-Higgins (Great Britain) reviewed developments in the interpretation of the concept of the chemical bond since 1948, when this subject was [last] discussed at an annual meeting of the French Physicochemical Society.

Longuet-Higgins presented data on the application during the past 5 years of mathematical methods to the study of hydrocarbons with conjugated bonds and of other molecules containing mobile electrons. The resemblances and differences between systems with localized electrons were outlined very clearly by Longuet-Higgins. In discussing the classification of bonds according to types, Longuet-Higgins stressed the necessity of differentiating between ionic or covalent bonds and those of a third type, i.e., bonds which are deficient in electrons, because their electrons are mobile, being nonlocalized or semi-localized. The concept involved here can be expressed by the theory of resonance between canonical structures or by the theory of molecular orbits which embrace several atoms simultaneously.

In discussing the two basic methods for interpreting the nature of the chemical bond, that of valency bonds and that of molecular orbits, Longuet-Higgins indicated that both methods result in the same proximate wave functions. However, these methods use entirely different concepts and are often regarded as competing with each other. Until recently, it had been assumed that the method of valency bonds is best for representing molecules with

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localized bonds, while the method of molecular orbits is most suited for conjugated systems and for metal crystals in which electrons move freely.

The possibility of representing the wave function of the molecular orbit of methane in two different ways had already been pointed out by C. Coulson. The first method corresponds to the concept of valency electron orbits which spread over the whole molecule; the second to a configuration in which two electrons are attached to every CH bond.

In his report, Longuet-Higgins showed a definite preference for the method of molecular orbits. His attitude toward the resonance theory is interesting. In discussing conjugated systems, Longuet-Higgins remarked that the resonance theory has been and is still used by organic chemists in interpreting the reaction capacity of conjugated systems as a function of their chemical structure. He then said: "Up to the present, the resonance theory has been the only general theory by means of which changes in the properties of molecules that depend on changes in the structure were interpreted. However, the resonance theory can hardly be regarded as a logical extension of the theory of valence bonds; it is essentially an intuitive simplification of the latter. It has now been demonstrated that the theory of molecular orbits yields applicable results for rather complicated structure with less trouble than the theory of resonance without the necessity of making approximations other than those which are inherent in the method."

In conclusion, Longuet-Higgins expressed the opinion that, at present, both theories are of equal significance for clarifying the interrelationships between the principal characteristics of the molecular structure and those of the chemical bond.

Participating in the discussion of Longuet-Higgins' report were R. S. Mulliken (US), R. Daudel (France), Mueller (West Germany), B. Pullman (France), J. W. Linnett (Great Britain), N. V. Belov (USSR), A. Laforge (France), E. Boyer (France), L. P. Orgel (Great Britain), E. Bergmann (Israel), and K. Frenkel (France). It is significant that, during the discussion which developed, practically no attention was paid to the theory of resonance of valency structures. This shows that the interest in this theory has declined.

On the other hand, one should note the considerable interest which French chemists evince toward the discussion which has developed in the USSR on basic problems of the chemical bond and of the theory of structure of organic compounds. This is demonstrated by "The Remarks on the Concept of the Chemical Bond," published by the French Center of Theoretical Chemistry; by the translation and publication of a number of articles written by Soviet chemical scientists (Questions Scientifique, Chimie, Vol 3, 1953); and by the publication of the article "Evolution, Since the Beginning of the 19th Century, of Ideas on the Structure of Matter and on the Meaning of Organic Chemical Formulas," by P. Rumpf (Pensee, No 41 and 44, 1952), in which considerable attention is paid to material pertaining to the Moscow conference.

The report by Longuet-Higgins and the discussion of his report completed the work of the Paris meeting on fundamental theoretical questions bearing on the nature of the chemical bond. The other reports presented at the meeting dealt with physical methods of investigation of the structure of molecules.

Professor L. E. Setton (Great Britain) in his paper reviewed progress in the investigation of the structure of molecules by the method of electron diffraction in gases.

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Professor R. Mecke (West Germany) presented a report entitled "Progress in the Field of Molecular Spectroscopy," and E. Roubine (France) gave a report entitled "Microwave Spectroscopy."

P. P. Shorygin commented on Mecke's report and presented an account of his own work dealing with the investigation of the intensity of lines of Raman spectra and with Raman spectra in the regions of absorption. In connection with this, a lively discussion on Raman spectra developed. The interest elicited by Shorygin's report was shown by the great number of questions asked of Shorygin during and after the meeting.

Engineer E. Grison (France) presented a report entitled "Localization of Hydrogen Atoms in Crystal Structures," and N. V. Belov gave an account of the work of Soviet scientists in this field.

Professor Y. Cauchois (France) gave a report on X-ray spectra.

Professor P. Grivet (France) reported on magnetic nuclear resonance, and B. M. Kozyrev (USSR) reported on magnetic electron resonance. Paramagnetic resonance absorption was discovered in 1944 by the Soviet scientist Ye. K. Zavoytskiy. Up to now, several hundred papers on paramagnetic absorption have been published. A review of this work was given by Kozyrev, who is a pupil of Zavoytskiy. Kozyrev's detailed report received much attention. Members of the audience asked many questions on the application of paramagnetic resonance in chemical investigations.

The meeting ended with a report by E. Lederer (France) on the application of chemical methods and particularly of physical methods to the determination of the structure of naturally occurring organic compounds. After the meeting ended, the Soviet scientists visited the laboratories of Irene Joliet-Curie, Professor C. Prevot, Professor J. Dupont, and Professor J. Mathieu. They also inspected the mineralogical laboratory directed by Professor P. Villiard, the X-ray laboratory (directed by Professor J. Mering) of the Chemical Research Center of the Ministry of Commerce and Industry, and the radiophysics laboratories directed by Professors P. Grivet, R. Daudel, and others.

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